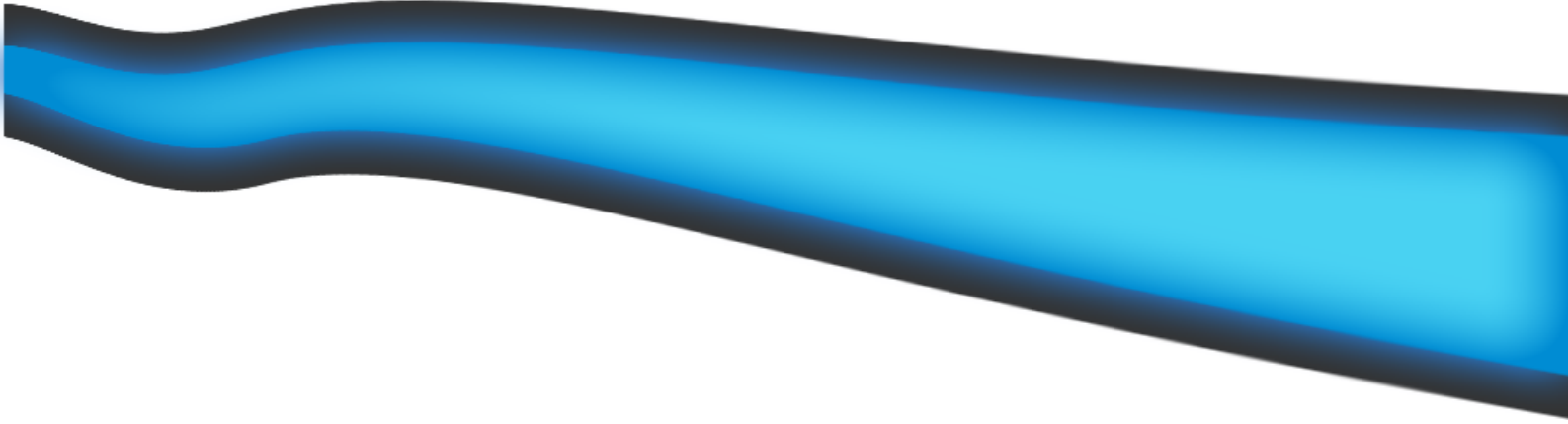

SECIL

Software Engine for
Configurations of Ionic Liquids

User's Guide

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1 Overall Purpose

Creating starting structures is a crucial task for any molecular modelling and is very difficult to evaluate *a priori*. For ionic liquids, which are amorphous condensed materials composed solely of (molecular) ions, the most "correct" starting structures – leading to the deepest minima the fastest, are difficult even to imagine. Furthermore, in the search for the most "correct" one there is an obvious risk of bias from the researcher.

SECIL uses a "mindless" algorithm to efficiently sample possible starting structures, configurations, for ionic systems, taking into account the packing of cations and anions, and automatically parses these to input files for popular computational chemistry packages.

We hope that the easy use of SECIL to construct molecular level models will benefit the ionic liquids community at large, and not be limited to computational studies.

2 Installation Instructions

2.1 Requirements

Before you try to install SECIL be sure that your computer system fulfils all necessary requirements as outlined below.

2.1.1 Java

SECIL is a Java application. To run properly on your system, it is necessary to have an updated Java Runtime Environment (JRE) installed, currently at least JRE 6. The JRE is not included in the SECIL data files. You can get a copy of the JRE at *java.com*.

2.1.2 OpenGL + JOGL

SECIL uses the advantages of OpenGL to create a user friendly working environment, thus make sure that your graphic card supports OpenGL. If you are not sure, just install the most recent drivers for your graphic card and take a look at the instructions if they are supporting OpenGL. In general all new graphic cards support OpenGL.

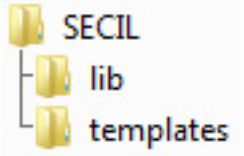
Java applications need the Java OpenGL (JOGL) libraries to display OpenGL content. SECIL is distributing different versions for Mac, Linux and Windows Operating Systems. The newest version is available at *https://jogl.dev.java.net/*. Download the correct files for your system (Windows, Mac, Linux, etc) and unpack them, modify your CLASSPATH environment variable to include the full paths to jogl.jar and gluegen-rt.jar:

```
"C:\Users\myhome\jogl-[version]-windows-i586\lib\jogl.jar"
```

Copy the jogl.jar as well as the gluegen-rt.jar to the SECIL/lib folder. The lib folder also provides some JOGL libraries which you can use.

2.2 Installation

SECIL is delivered as Zip archive for different operating systems (Windows, Mac and Linux). After downloading SECIL for your Operation System, unpack the zip file and you get the following folder structure:



To install SECIL permanently copy the SECIL root folder to a proper location on your hard drive *e.g.:*

"C:\Program Files\SECIL"

The SECIL folder contains a Java archive file *SECIL.jar,* that contains the basic SECIL software. The lib folder is keeping the molecule library for the program (lib.xml) and a sub-folder, containing a System dependent version of the necessary OpenGL Library files. To Install SECIL properly, read and follow the OpenGL instructions in c*hapter 2.1.2* carefully. Make sure to unpack the OpenGL library files into a folder on your hard drive (see chapter 2.1.2) and link your System CLASSPATH to the library file location.
Also create a copy of the two files *jogl.jar* and *gluegen-rt.jar* in the "`../SECIL/lib`" folder.

3 Getting Started

3.1 GUI

Figure 1 shows the basic Graphical User Interface (GUI) of SECIL with its three main working elements, the Library 1, the active area 2 and the Results tree 3.

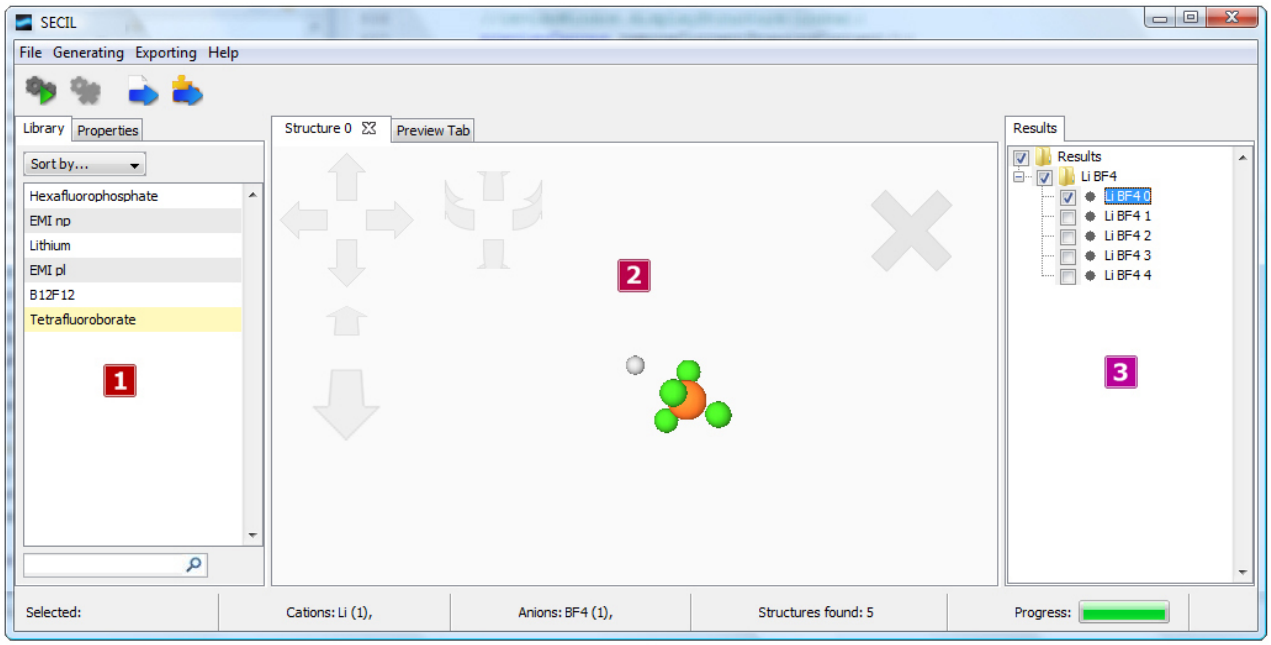


Figure 1: The Graphical User Interface.

3.1.1 Library

The library is divided in a list, a sorting menu and a search field. The list displays the individual entries stored in the library file. When you start SECIL the list is sorted chronological from top to bottom and whenever you import a new entry, it is displayed at the bottom of the list.
You might want to sort the list alphabetically or by charge, thus you use the drop down menu, which is located above the list saying "*Sort by...*".
If you cannot find a particular entry, but you know that it is included, find it by typing its name, a sub-string of it or even only the first letter into the search field. Since the search field is directly connected to the list, the search results will appear immediately. To display all entries again, just erase the search expression.

3.1.2 Active Area

You find the active area n the center of SECIL's GUI. Figure 1 shows a 1:1 ion pair of lithium (Li) and tetrafluoroborate (BF_4) in 3D. Located in the top left and right corner of the 3D display are buttons to move (x, y, z dimension), rotate or remove a single molecule. Multiple displays are managed by tabs. You can switch from tab to tab to focus different active areas.

3.1.3 The Result Tree

The result tree arranges the generated configurations as shown in Figure 1. Every time a configuration generation is finished, a new folder node containing the seperate configurations is created and displayed in the result tree, with an appropriate name due to the included ions/molecules etc. You can collapse a folder by doubleclicking it and open it the same way.

4 Library Maintenance

4.1 Importing

SECIL includes a couple of entries (ions/molecules) in its library by default, to allow you to explore its possibilities without importing your own. However, most likely you will eventually want to use a set which is not listed in the current library. Therefore, you can import as illustrated in Figure 2. Select "*File → Import*" in the main menu. 1 Here you have the choice to import a Spartan file, which is generated by the Titan/Spartan molecule modelling software[1] or a XYZ-File[2]. Select the data file, which you want to use, via the file chooser. As seen in Figure 2 the new molecule is displayed on the screen and a property panel blends in where the library tab used to be. 2 Enter a proper name, an abbreviation and the correct charge of this entry (you can change the properties later at any time). After specifying the properties, click "Add to Library". Afterwards the new entry is displayed in the library list 3. Now it is ready to use (see Adding Molecules).

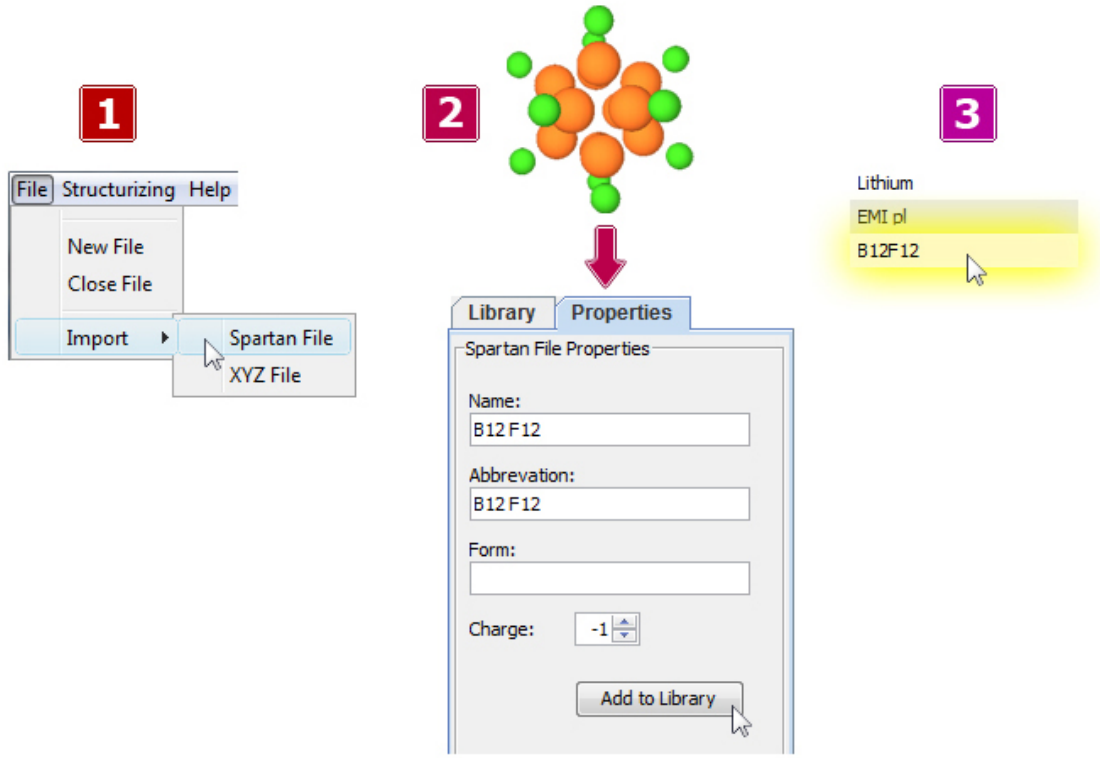


Figure 2: Adding a new ion to SECIL's library

To avoid duplicates, SECIL checks if the same ion/molecule is already included in the library and if the chosen name/abbreviation is occupied. A dialogue informs you.

For consistency and correct functionality only add separate ions/molecules as entries i.e. no pairs or higher aggregates.

1 *Titan*, 1.0.1; Wavefunction Inc. and Schrödinger Inc.: Irvine CA and Portland OR, 1999.
2 See Appendix A

4.2 Deleting Library Entries

There are two ways to delete a entry from the library:

a) Via the popup menu: right-click on the name in the library list and you get the option "*Delete*" 1. Select and accept the safety dialogue by pressing "*Yes*" 2 (Figure 3).

b) Open the molecule in a display tab (see Adding Molecule), select it 1 to open the properties panel. Click the "Delete" button 2 as shown in Figure 3. A safety dialogue asks for confirmation 3.

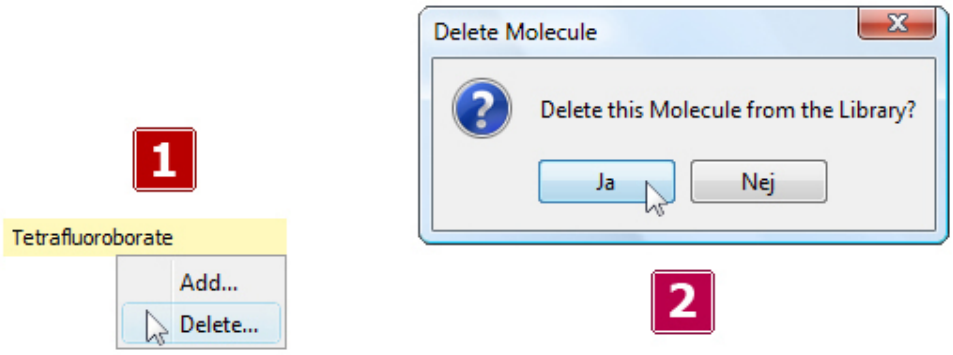


Figure 3: Deleting an unwelcome entry from the library

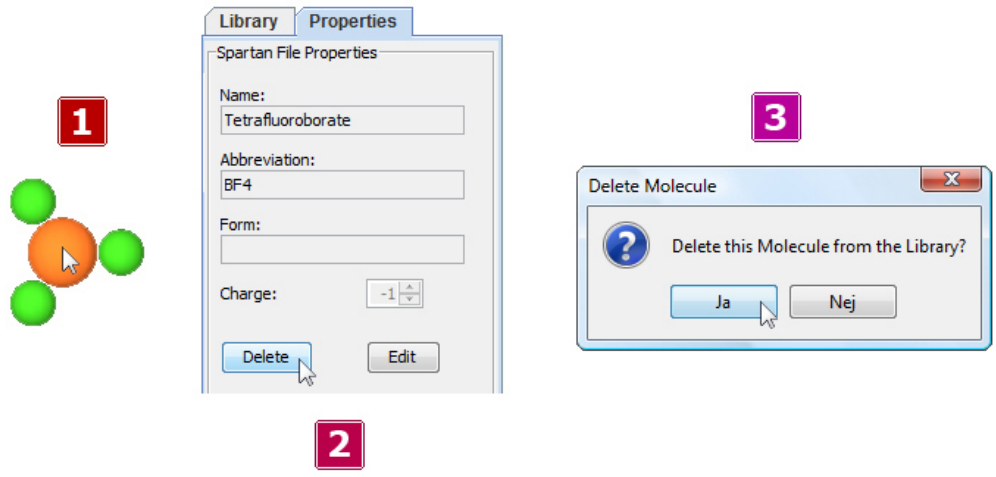


Figure 4: Deleting an entry using the properties panel

4.3 Editing Properties

Every library entry is editable: name, abbreviation, form and charge. Figure 5 illustrates the steps to change the properties. After adding a molecule to the screen, select it 1 by clicking on it. The properties panel appears. Now use the "*Edit*" button 2 to enable the input fields. After editing the corresponding fields, you can save the data by clicking the "*Save*" Button 3. After saving, the library and every other instance of this entry is updated immediately.

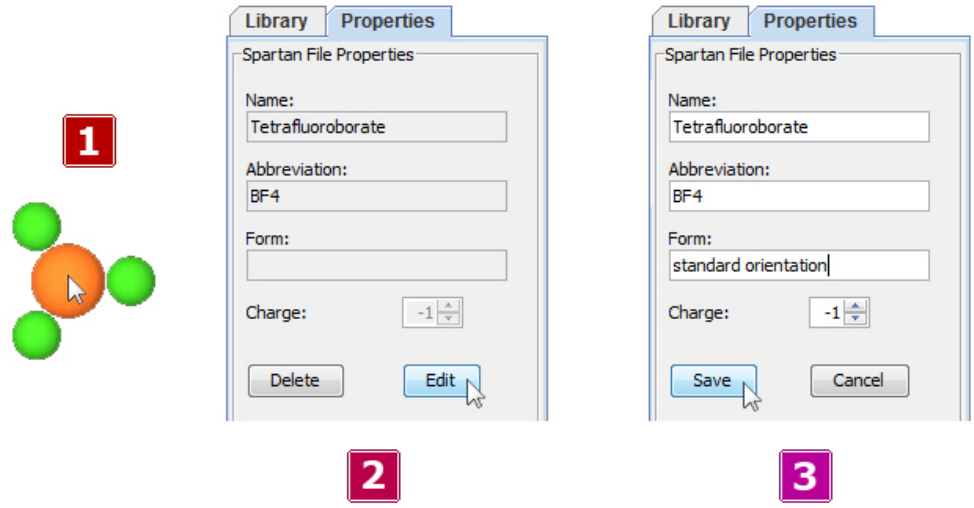


Figure 5: Editing the entry properties

4.4 Sorting and Searching

In case you can not find a specific entry in the library list, you have two options, which will help you. First, you can sort the list alphabetically or by charge, where the entries are split in cations and anions (see Figure 6). To sort the library click on the "Sort by" choice box, now select either "*Charge*" or "*Alphabetical Order*".

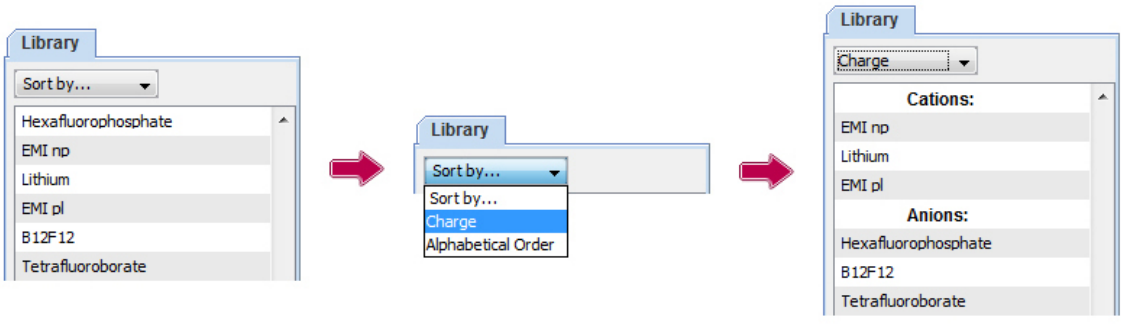


Figure 6: The library before and after sorted by charge

Second, you can look up the entry directly by typing its name in the search field. The field is case sensitive. The search function starts as soon as a single character is entered in the search field, usually it is enough with a subsequence of the given name. Figure 7 shows a search for the lithium ion. All matches, containing a subsequence of the entered sequence, will be displayed in the list. You can reset the library list by clearing the search field.

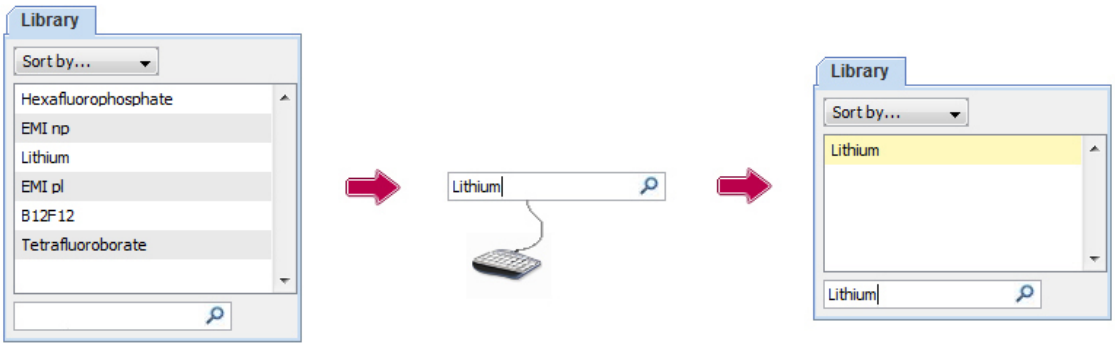


Figure 7: Looking up lithium using the search function

Tip: When you are looking for a family of chemical compounds (e.g. imides), just type "imide" in the search field. This is a convenient starting point to create various imide-based configurations.

5 Configuration Generation

5.1 Adding Ions/Molecules

A configuration is built directly from library entries. The library list displays all the accessible entries (ions/molecules). You can add a entry to a new or existing by double clicking on its name. In case no display tab is selected, a new display tab will be created, including the selected entry(s).
If you want to add more than one molecule of the same kind, it is more convenient to right click on the entry name and choose "*Add...*" 1 in the popup menu. A dialogue will appear. After specifying the amount n, press "*Add*" 2 to insert n entries to your working configuration. All entries will be displayed in the same display tab 3 . Cancel the dialogue by pressing Cancel.

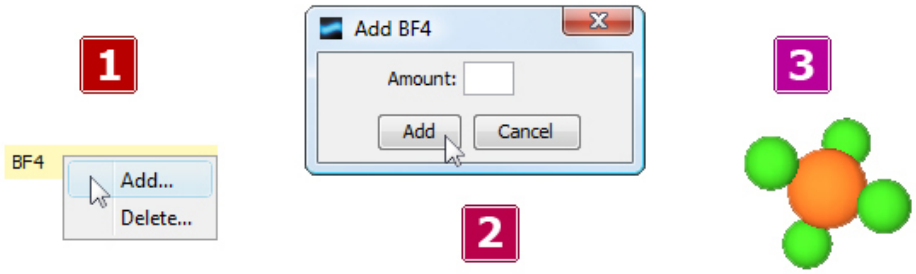


Figure 8: (1) the popup menu selected is "Add..", (2) the add- dialog, (3) a displayed molecule

5.2 Removing Ions/Molecules

To remove an ion/molecules from a configuration by using the remove button in the upper right corner of the active area. Select the particular molecule 1 by left-clicking with the mouse, followed by pressing the Remove button 2 . The status bar shows the updated amount of entries for the active configuration.

Figure 9: Deleting a molecule from the configuration

5.3 Generating Configurations

A set of configurations based on the active area can be generated if at least one anion and one cation entry exists. The status bar gives information about how many and which entries currently are active.
Start the generation of configurations by selecting "Generating → *Run...*" in the Main menu or by clicking the Generate button in the toolbar 1 . A setup dialogue appears to allow you to decide on the number of configurations. Click on the check box, type a number in the input field, and accept by clicking on the "*Generate*" button 2 .
The generation process starts. During this process, the active area is locked 3 until all configurations are generated (or you press the "*Cancel*" button to cancel the process). Upon successful generation a list of the resulting configurations is displayed in the result tree 4 . Figure 10 schematically shows all the necessary steps to generate configurations.

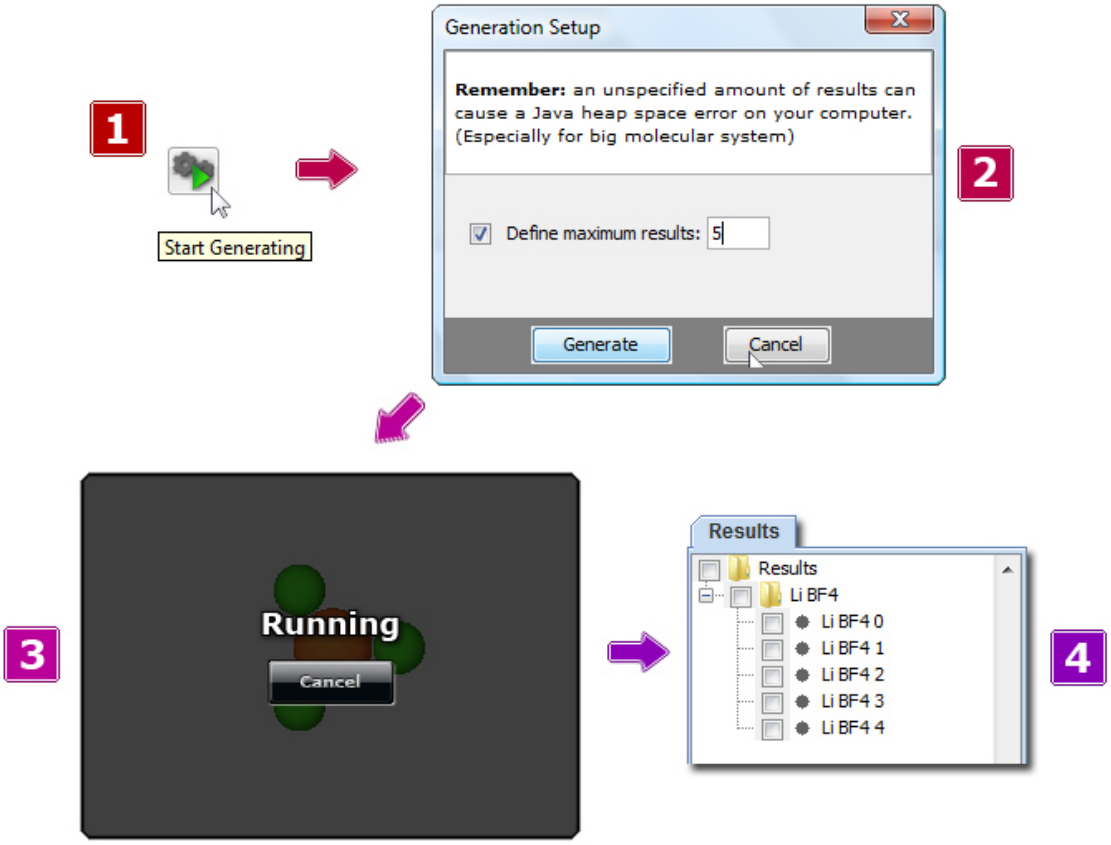


Figure 10: Guiding through the different structure creation steps

Remember: The computational effort of configuration generation rapidly increases with the number of entries and number of configurations specified. Do small test runs first.

5.4 Renaming Configurations

By default configurations are named on the entries included. This naming may not be the best. You can easily rename your set of configurations by a right-mouse-click on the group folder 1. An input field shows up, where you can enter a new name 2 (Figure 11).
All configurations in this folder will be updated with the new names automatically 3.

Figure 11: Renaming set of configurations

5.5 Previewing Configurations

By double-clicking on a specific configuration in the Result tree, the Preview Tab opens up and the selected configuration is displayed. You can now scan through the configurations within the folder by using the arrow keys ↑ ↓.

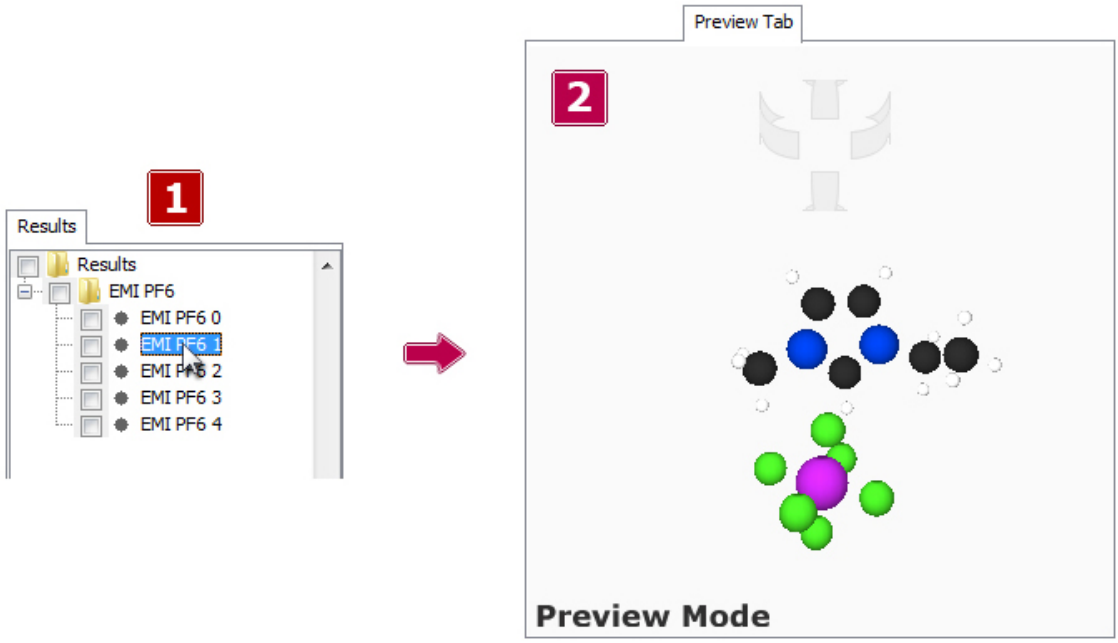


Figure 12: Selecting a structure and previewing it on the screen

You can mark each result by pressing x.

6 Configuration Exporting

6.1 Exporting your Configurations to Gaussian03/09

There are two ways to create Gaussian input (and setup) files from your generated configurations: either by using a wizard or an editor.
The export wizard allows you to follow a step by step procedure and provides a fast solution, but is quite limited in possibilities. The export editor is more advanced and versatile; You need to know Gaussian03/09 input file syntax and if applicable, also the syntax of the cluster manager of your computer system (for setup files).
Common to both paths to exporting is that you first select the folder and the specific configurations you want to export by using the check boxes (Figure 13). Then you either open the Export Wizard or the Export Editor , by clicking on their icons in the toolbar or by using Main menu "E*xporting → …*" .

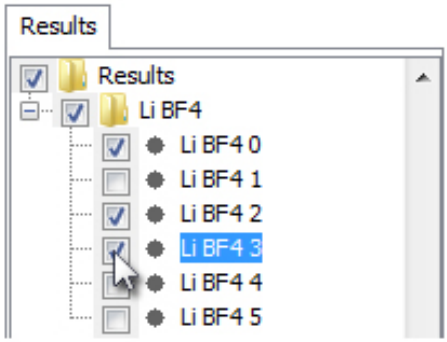


Figure 13: Selecting configurations in the result tree

6.2 Export Wizard

The exporting wizard consists of three input screens for user, cluster and file information:

1. User Information:
Here you specify a valid email address. Depending on system this might allow you to receive information about the status of a job, *e.g.* when it is started, finished or cancelled. Here you can also load complete templates, from previous exports.

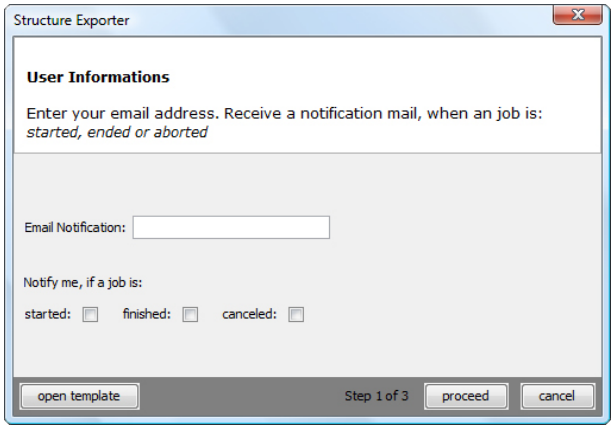


Figure 14: Export Wizard - The User Information Screen

2. Cluster Information:
Most tasks on supercomputers or clusters are managed by cluster managers. Currently PBS and SLURM are supported. It is necessary to enter your account name of the particular cluster. You also specify here wall-time, number of nodes, cores and memory for your runs. The default values are: Wall-time = 45 min, Nodes = 1, CPUs = 4, Memory = 1024 MB.

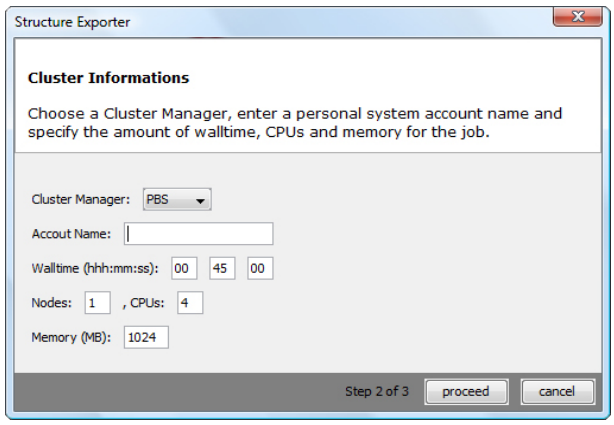

Structure Exporter
Cluster Informations
Choose a Cluster Manager, enter a personal system account name and specify the amount of walltime, CPUs and memory for the job.
Cluster Manager: PBS
Accout Name:
Walltime (hhh:mm:ss): 00 45 00
Nodes: 1 , CPUs: 4
Memory (MB): 1024
Step 2 of 3
proceed
cancel

Figure 15: Export Wizard - The Cluster Information Screen

3. File Information:
This is the Gaussian specific route line information. You choose an algorithm and and a basis set to combine with. The two check boxes "*Freq (Raman)*" and "*SCF(Tight)*" are enabling a Raman spectrum calculation and a tight SCF convergence respectively.
In the comment line you may want to enter a personal note about the calculation.
Finally you have to select a folder for saving the exported input files into.
You can also save the completed data in a template file by using the "Save Template" button.

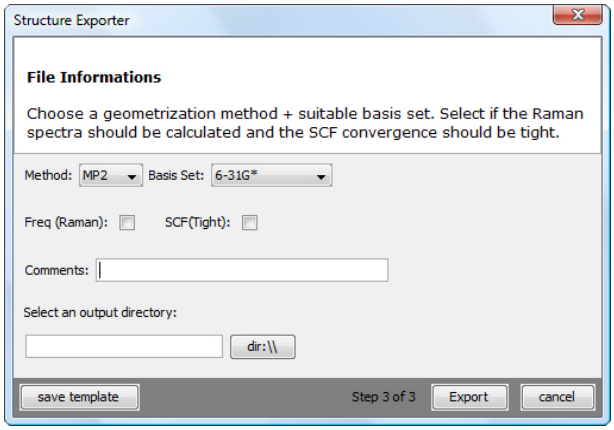


Figure 16: Export Wizard - The File Information Screen

6.3 Export Editor

The Export Editor allows you to create detailed input files and if necessary cluster manager files. In Figure 17 you see the icons New , Open , Save and Cluster Setup .

Creating Files

The content for the GAUSSIAN setup files is to be entered in the text area of the *Gaussian Input* tab. In most cases you need to create an Cluster manager information file as well. Thus click the *Cluster Setup* icon 1 in the toolbar to enable the *Cluster Manager Info* tab 2.
It is often required to add the file name into your files, e.g. for a check file which is created by GAUSSIAN. Hence you can click the <F> icon and a [FILENAME] text mark will appear in between the data. This token, used at the right position, will change to the real file name during the exporting process.
In the end of the data add a single blank line by pressing the enter button on your keyboard. SECIL will auto complete the files in the exporting process.
You find the GAUSSIAN syntax at their website[3]. Look up the manual pages of the cluster manager for the corresponding syntax.

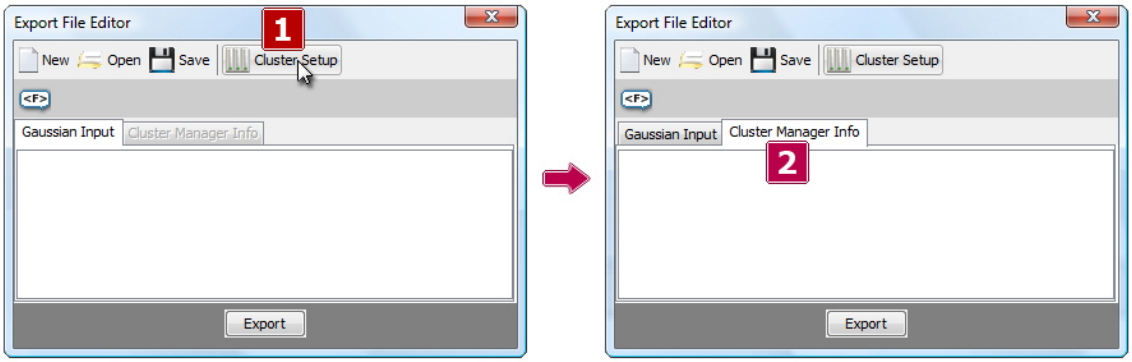


Figure 17: The Export File Editor

To prevent of losing content, save the files you are working on, before you use the New file function.

3 Gaussian '09 documentation: http://www.gaussian.com/g_tech/g09ur.htm

7 Additional Information

7.1 About SECIL

SECIL was created at Applied Physics, Chalmers University of Technology in Göteborg, Sweden.

The SECIL project, software creation and first examples of usage, was made possible by a grant from "*Stiftelsen J. Gust. Richert*" to Dr. Patrik Johansson 2009-2010, which is most gratefuly acknowledged.

SECIL is written in Java and ifreeware.

7.2 About the Creators

Knut Angenendt studied computer science at the Carl von Ossietzky University of Oldenburg, Germany. He wrote his diploma thesis at the Chalmers University of Technology in Göteborg, Sweden. After graduating he was employed by Chalmers to work on the SECIL project. He has written all the code, developed all the algorithms and the software design of SECIL.

Dr. Patrik Johansson is Assoc. Prof. at Applied Physics at Chalmers University of Technology. One of his major research areas is the physics of ionic liquids, especially for applications such as electrolytes for batteries and fuel cells, and more specifically the role of the ion-ion interactions. He initiated the SECIL project with the main idea and aims.

8 Appendix A

8.1 XYZ File Format

"The XYZ file format is a chemical file format. There is no formal standard and several variations exist, but a typical XYZ format specifies the molecule geometry by giving the number of atoms with cartesian coordinates that will be read on the first line, a comment on the second, and the lines of atomic coordinates in the following lines. The file format is used in computational chemistry programs for importing and exporting geometries. The units are generally in Ångströms. Some variations include using atomic numbers instead of atomic symbols, or skipping the comment line. Files using the XYZ format conventionally have the .xyz extension."[4]

Example (1-ethyl-3methyl imidazolium):

```
19
EMI
N        0.620630    0.022983   -0.318667
C       -0.411529   -0.817348   -0.205078
N       -1.522548   -0.114765    0.040034
C       -1.187244    1.225362    0.086113
C        0.152686    1.310602   -0.136832
C        2.032814   -0.363533   -0.558705
C        2.888449   -0.253520    0.698027
C       -2.871754   -0.668959    0.223378
H       -0.358686   -1.889826   -0.299841
H       -1.922264    1.992996    0.264387
H        0.802133    2.168870   -0.187044
H        2.403989    0.277985   -1.359356
H        2.015852   -1.383817   -0.943528
H        3.911193   -0.552743    0.460513
H        2.522202   -0.907467    1.491975
H        2.924043    0.769143    1.079038
H       -3.238362   -0.414594    1.216938
H       -2.828362   -1.751144    0.121609
H       -3.538834   -0.262554   -0.535675
```

4 Source: http://en.wikipedia.org/wiki/XYZ_file_format